Data Dictionary

Journal Article to be Published:
Inactivation of Bacillus Spores in Wash Waters Using Dilute Chlorine Bleach Solutions at Different Temperatures and pH Levels

Clearance Tracking Number:
ORD-017617

Authors:
Vicente J. Gallardo, Donald A. Schupp, John L. Heckman, E. Radha Krishnan, Eugene W. Rice

1.0 Introduction

The source for all the data in the published article can be found in the Excel spreadsheet entitled "inactivation data.xlsx"

The following distinctions are helpful in understanding this document. The term "spreadsheet", in this case, refers to the entire Excel spreadsheet that contains all the data found in the journal article. The term "worksheet" refers to individual pages of the Excel spreadsheet. The Excel spreadsheet contains numerous worksheets.

This present document explains the above mentioned spreadsheet, heretofore referred to as "the spreadsheet". In addition, this document explains where the data in the published figures and tables can be found in the spreadsheet.

2.0 Tables

The published tables (Tables 1 – 5) are included in the spreadsheet. Each of these tables can be found in the spreadsheet as a unique worksheet and labeled appropriately. For example, Table 2 can be found in the spreadsheet in the worksheet labeled, "Table 2". The worksheets for Tables 1 - 5 are at the beginning of the spreadsheet. To aid in explaining the data, the versions of the tables found in the spreadsheet have additional columns not found in the published tables.

The following describes the individual Tables 1 – 5 that can be found in the spreadsheet.

Table 1. Description of Wash Waters Studied

For the purpose of publishing the journal article, the wash waters were designated by a letter, e.g., A, B, C. During the research effort the wash waters were designated in a different fashion. The version of Table 1 that can be found in the spreadsheet cross references the two ways that were used to designate the wash water. The original designation can be found in column D of this worksheet.

Table 2. Water Quality Parameters of Wash Waters

This table is a summary of the initial characterization of the wash waters tested. Table 2 also includes additional information not found in the published version to help explain the data. The version of Table 2 that can be found in the spreadsheet cross references the two ways that were used to designate the wash water. The original designation can be found in column G of this worksheet. Table 2 is a simplified version of the data found in the worksheet entitled "Initial Char.", which has additional information, e.g., date water was generated.

Table 3. General Inactivation Results. 3,000 mg NaOCl/liter

This contains the bulk of the summarized inactivation data for the journal article. Each row of data in this table (except for those that are marked as "average") contains results from a unique inactivation test. The version of Table 3 in this spreadsheet includes a column (Column "B") that gives the number of each individual test. (This column is not shown in the published version.)

As an example, for the tests at ~20°C, wash water A (floor wash water with Alconox), the individual test numbers are 1a, 1b, and 1c. The inactivation results for each individual test can be found in an individual worksheet labeled to correspond to the test number. For example, for test # 1a, the results can be found in the worksheet labelled 1a.

Table 4. Inactivation at Different Amounts of Contact Time Before Adding Chlorine Bleach

Tables 4 also contains inactivation data and also has a column (Column "B") that gives the number of each individual inactivation test.

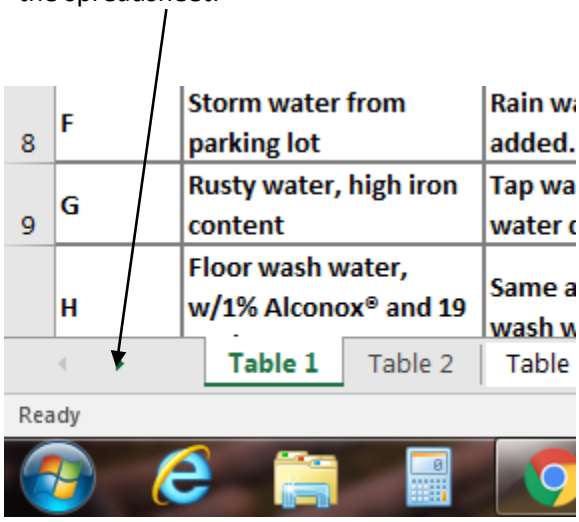
Table 5. Inactivation Results in Non-buffered and Buffered Car Wash Water w/1% Dawn®

Tables 5 also contains inactivation data and also has a column (Column "B") that gives the number of each individual inactivation test.

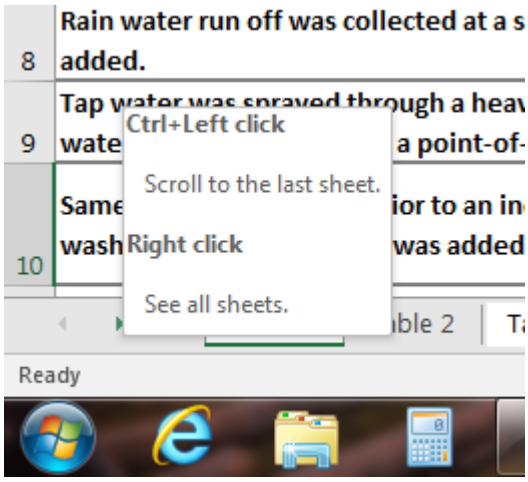
3.0 Description of Worksheets with Data from Individual Inactivation Tests

The spreadsheet has many individual pages (worksheets) To ease navigation through the spreadsheet, the following hints may be helpful if using Micrsoft Excel:

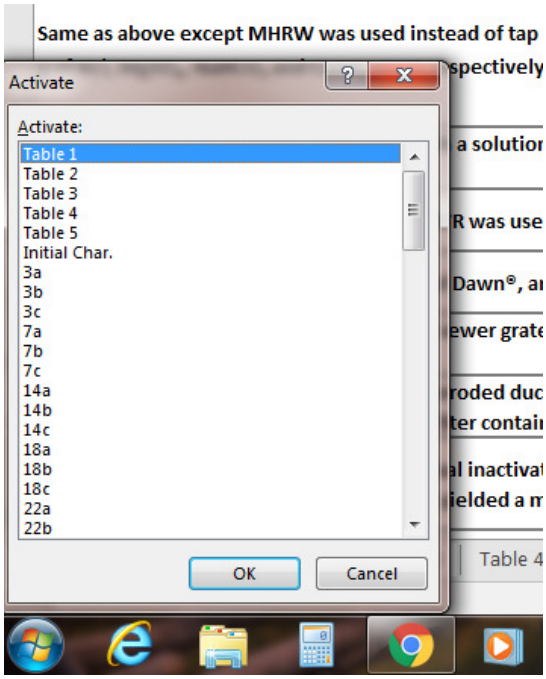
1. Allow cursor to hover in bottom left hand corner of the spreadsheet:



2. A dialog box should pop up as shown. Right click to see a list of all worksheets



3. Select worksheet to view and double click to view it.



The following describes the data contained in the individual worksheets that contain the inactivation data from the individual tests.

For reference, the reader should be in cell A1 when going through the following description.

The first ~16 rows of the worksheet contain the conditions of the test (date, test #, washwater type (abbreviated WW), and the recipe used, i.e., the volume of wash water, the amount of bleach, spores and buffer added.) The resulting bleach concentration in the reaction vessel is given, typically in cell B15 or B16. This is the concentration used in calculations for the value of CT referred to in the published article.

Most of the data in these individual worksheets are self-explanatory from the column heading. The following provides more information.

Going from left to right in the worksheet that contain data from individual inactivation experiments:

Column A. *Time*
Sample time, in minutes, of the inactivation experiment.

Column B. *Temp(°C)*
This contains the temperature during inactivation. For the purposes of the article, the average temperature was reported. Not all the data in this column were used to calculate the average. The temperature prior to chlorination was not included. In addition, the only temperature measurements included in calculating the average were ones where an actual amount of inactivation could be calculated. That is, if complete inactivation had occurred (no colonies on any plates for that sampling point) the corresponding temperature measurement was not included. The average temperature is shown at the bottom of this column of data.

Column C. *pH (WW)*
This refers to the pH during inactivation. The pH at time 0, shows the pH before chlorine addition. These values of pH are also the ones shown in Tables 3, 4 and 5 under "pH of the water". The other measurements in this column in the worksheet show the pH after chlorine addition. These values of pH are also the ones shown in Tables 3, 4 and 5 under "pH after Cl_2 addition."

As with the temperature data mentioned above, for the purposes of the article, the average pH after chlorine addition was reported. The only pH measurements that were included in calculating the average were from samples where an actual amount of inactivation could be calculated. The average pH is shown at the bottom of this column of data.

Column D. *pH (Sample)*
This refers to the pH of the quenched samples. To halt inactivation, the samples were quenched with sodium thiosulfate.

Column E. *Free Cl (mg/L) (WW)*
This shows the concentration of free chlorine at the corresponding time of inactivation. Due to the high dilution required prior to chlorine measurement, this data occasionally had much variability and thus was not used in the calculation of the CT values.

Column F. *Free Cl (mg/L) (Sample)*
This shows the concentration of free chlorine after quenching with sodium thiosulfate.

Column G. *Turbidity (NTU)*
This shows the turbidity of the water at a given time.

Column H . *COD (mg/L)*
This shows the chemical oxygen demand (COD) of the water at a given time.

Column I . *B. globigii Conc./100 mL*
This column shows the concentration of *B. globigii* (Bg) in the wash water per 100 ml of sample.

Column J*. LI*
The column immediately to the right of the column showing the Bg concentration is the amount of log inactivation (LI) at the corresponding time. If there was complete inactivation, then the LI value is expressed as a "greater than" value.

Column K*. HPC Conc./ 100 mL*
In addition to Bg analysis, total Heterotrophic Plate Counts (HPC) were also measured. Viable Bg spores also showed up as counts in the HPC analysis. This data was not used in the article but served as a check for the Bg data.

Column L. *LI*
The column immediately to the right of the column showing the HPC concentration is the amount of HPC log inactivation (LI) at the corresponding time. If there was complete inactivation, then the LI value is expressed as a "greater than" value. This data was not used in the article.

Column M. *TSS (mg/L)*
This shows the total suspended solids (TSS) of the water at a given time.

Column N . *TDS (mg/L)*
This shows the total dissolved solids (TDS) of the water at a given time.

Column O*. Alkalinity (mg/L)*
This shows the total alkalinity (TDS) of the water at a given time.

Column P. *Ct*
This refers to the chlorine concentration (C) multiplied by the contact time (t). This is abbreviated as CT in the journal article. This was calculated by multiplying the applied dose of chlorine, expressed as mg/L of NaOCl, by the contact time in minutes. Ct values were only calculated for sample points where there was a finite amount of inactivation occurring. If there was complete inactivation, then no Ct value is given.

Column Q. *Ct for 6 log kill*
The value in this column is the calculated Ct needed for 6 log kill, this parameter is expressed as CT_{6log} in the article. This data was calculated by first conducting a linear regression of the data in the plot of log inactivation versus Ct. (This plot is also shown in each of the individual worksheets). The slope was determined and then to calculate the time needed for 6 log kill, the following equation was used:

Ct for 6 log kill = 6/[slope of linear regression]

Column R. *time for 6 log kill in 3,000 ppm Cl2 (minutes)*
This gives the time needed to effect a 6 log kill at a disinfectant concentration of 3,000 mg/L disinfectant. This parameter is expressed as T_{6log} in the article. The value of the parameter was calculated from the above value for Ct for 6 log kill and dividing by 3,000:

T_{6log} = Time for 6 log kill in 3,000 ppm = Ct for 6log kill/3000

Column S. **time for max log kill @ working concentration*
This is an artifact of some calculations that were not used in the data analysis described in the journal article.

4.0 Figures.
The data used for the figures in the article are described in the following section.

Figure 1. Examples of Log Inactivation vs. CT Plots
This graph shows the amount of inactivation for selected experiments relative to CT. The data can be found in the spreadsheet in individual worksheets denoted in the following table.

Data series in Figure 1	Worksheet in spreadsheet, Inactivation Data.xls
Floor wash water w/Alconox® and motor oil;	20aR
Stormwater 4°C	20c
Stormwater 21°C	9c

Figure 2. Time for 6 log kill vs. pH, After Cl_2 Addition, Room Temperature
The data from this graph were taken from Table 3. The average values for time for 6 log removal (T_{6log}) and pH were used in the plotting of this graph.

Figure 3. Time for 6 log kill vs. pH, After Cl_2 Addition, 4 °C
The data from this graph were taken from Table 3. The average values for time for 6 log removal (T_{6log}) and pH were used in the plotting of this graph.

Figure 4. Free Chlorine Concentration vs. Time
This graph shows the results from free chlorine measurements over the length of selected inactivation experiments. The data can be found in the spreadsheet in individual worksheets denoted in the following table. The data for chlorine concentration are in the units of mg Cl2/liter and come from measurement of chlorine using the method described in the article (HACH. 1997. Instruction Manual for Free Chlorine Following DR/4000 Procedures, Loveland, Colorado, U.S.A.). The chlorine data points are in column E, and the time data points are in column A of the individual worksheets.

Data series in Figure 4	Worksheet in spreadsheet, Inactivation Data.xls
Car wash water, 21°C	10a
Car wash water, 4°C	21c
PPE washwater, 21°C	5a
PPE washwater, 4°C	16a

Figure 5. Time for 6 Log kill vs. pH. Results From Buffered and Non-buffered Car Wash Water, 4°C
The data from this graph was taken from Table 5, using the results from the experiments at 4°C.

Figure 6. Log inactivation vs. CT, With and Without an Apparent CT lag
This graph shows the amount of inactivation for selected experiments relative to CT. The data can be found in the spreadsheet in individual worksheets denoted in the following table.

Data series in Figure 6	Worksheet in spreadsheet, Inactivation Data.xls
buffered carwash water, pH = 7.00	21k
unbuffered carwash water, pH = 10.06	21l